Indene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 2.62 °C

Global applicability domain: Inside

Local applicability domain index: 7.82e-01

Confidence level: 4.84e-01

Nearest Neighbors from the Training Set

Image not found
Indene
Measured: -1.80
Predicted: 2.62

Image not found
1H-Indene, 2-methyl-
Measured: 80.0
Predicted: 16.8

Image not found
Indan
Measured: -51.4
Predicted: -17.3

Image not found
Cyclopropylbenzene
Measured: -31.0
Predicted: -15.7

Image not found
2,5-Norbornadiene
Measured: -19.1
Predicted: -22.9